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Addressing uncertainties in cap rock integrity assessment through a response surface methodology

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Abstract

This paper presents a methodology to develop simplified models to address uncertainties in cap rock integrity assessment to support decision making in the CO_2 storage risk management. Conventional analytical approaches might lead to a misestimation of cap rock failure, whereas conventional numerical approaches are too computer time-consuming regarding the multiple realizations required by an uncertainty analysis. An intermediate solution is then proposed based on the response surface methodology, consisting in estimating the stress state after CO_2 injection as a linear combination of the most influential site parameters. An uncertainty analysis methodology is proposed and illustrated on the Paris Basin case.

Keywords: CO_2 geological storage; Coupled hydraulical and geomechanical modeling; Tensile fracturing; Shear slip; Response surface method; Sensitivity analysis; Uncertainty analysis

1. Introduction

CO_2 capture and geological storage (denoted CCS) is seen as a promising technology in the portfolio of measures required to mitigate the effects of anthropogenic greenhouse gas emissions. Demonstrating safety constitutes a prerequisite to its large-scale implementation. Bouc *et al.* [1] describe the methodological framework developed to determine such safety criteria. The method is based on the identification of risk scenarios, which are represented by simplified models. To support an informed decision making, the objective is to study the effects of uncertainties in input parameters on the outcomes of the models.

Cap rock integrity constitutes one of the key aspects of safety. Compromising cap rock integrity could give way to leaks, hence potentially generating risks for the humans and the environment, and also decreasing, if not ruining, the efficiency of the storage to fight against climate change. This paper presents a methodology to develop simplified models to address such a geomechanical risk. The first part of the paper gives an overview of the numerical and analytical conventional approaches to investigate cap rock integrity. The limitations of both approaches are underlined regarding the simplicity and flexibility constraints required by the methodological framework for determining CO_2 safety criteria. In a second part, an alternative strategy based on the response

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surface methodology (Box and Wilson [2]) is described to develop such simplified models. A third part illustrates the use of the simplified models to address uncertainties in cap rock integrity assessment in the context of the French Paris Basin (based on the studies carried out in the PICOREF project [3]).

2. Caprock mechanical integrity assessment

Recent large scale coupled hydromechanical simulations (e.g. Vidal-Gilbert et al. [4], Rutqvist et al. [5]) have shown that the most important process in hydromechanical behaviour of the caprock during injection of CO_2 is an increase in the pore pressure reservoir leading to a general decrease in the effective stresses, which can be defined as follows (Terzaghi [6]):

$$\sigma'_{ij} = \sigma_{ij} - P\delta_{ij} \tag{1}$$

Where δ is the Kronecker symbol (δ_{ij}=0 if i≠j and δ_{ij}=1 otherwise) and σ is the total stress.

The most affected zone is located close to the injection well at the interface between the reservoir injection zone and the caprock layer. Such changes might lead to caprock failure and thus to a tremendous diminution of caprock integrity. Two mechanical failure mechanisms can occur during CO_2 injection, namely tensile fracturing and shear slip reactivation of preexisting faults depending on the principal effective stress (σ'_1; σ'_3) after injection.

2.1.1. Tensile fracturing

The potential for tensile failure is usually investigated under the conservative assumption that a tensile fracture could develop when the minimal effective stress σ'_3 becomes negative (under the soil mechanics convention) and its absolute magnitude exceeds the rock matrix tensile strength (denoted σ_T), which is usually assumed to be null. The tensile failure criterion is defined as follows:

$$\sigma_T + \sigma'_3 \leq 0 \tag{2}$$

2.1.2. Shear slip

The potential for shear slip along preexisting fractures is investigated under the conservative assumption that a cohesionless fracture could exist at any point of the studied zone with an arbitrary orientation. For such a case, the shear slip failure criterion (*i.e.* Mohr Coulomb criterion) can be written as follows:

$$\sigma'_1 - q\sigma'_3 \geq 0 \tag{3}$$

Where q is related to the fracture static friction angle of the fracture such that $q \approx 3$ when fracture static friction angle is 30° (Jaeger and Cook, [7]).

2.2. Numerical analysis

The effective stress state after the injection can be investigated by means of a numerical tool (typically the finite element method), which can take into account complex geological architecture, complex injection scenario, coupling between different physical phenomena and various types of rock materials… A typical numerical large scale coupled hydraulical and geomechanical model is described on Figure 1 to assess caprock integrity in the context of a multilayered aquifer such as the Paris basin.

2.2.1. Geometry and Boundaries description

The multilayered system consists of the reservoir (denoted in abbreviated form *res*), the caprock (denoted *cap*), the basement (denoted *bas*) and the overburden (denoted *ove*) formation. Figure 1 represents the geometry and the boundary conditions of the model. The plane strain condition is assumed. Vertical displacement at the bottom and horizontal displacement at the lateral boundaries are fixed. Hydraulic flow is set to zero at the bottom and lateral boundaries. The problem is solved in the framework of the saturated elastic porous media.

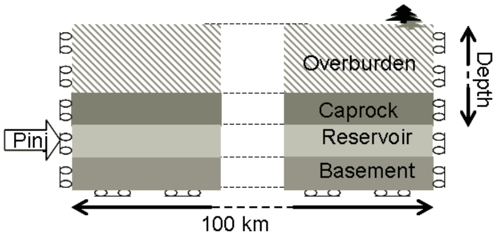

Figure 1: Typical large scale numerical model for cap rock failure risk assessment in a multilayered geological system

2.2.2. Model parameters

The mechanical behaviour of the rock matrix is elastic and governed by the Young modulus (denoted E) and the Poisson's coefficient (denoted υ). Hydraulical properties are defined by the intrinsic permeability (denoted k) and the porosity (denoted ω). The caprock and the reservoir formation thickness (denoted H_{cap} and H_{res}) both range from 50 to 150m in the context of the Paris basin. The rock mass is saturated and the initial Hydraulical condition is hydrostatic. The stress regime is extensional in the Paris basin with a ratio K_0 ranging from 0.5 to 1.0. Injection is conducted at a depth ranging from 1000 to 2000 m and is modeled by a gradual pore pressure increase during on eyear. The injection pressure is denoted P_{inj} and ranges from 1.25 to 3.0 times the initial pore pressure.

2.3. Conventional analytical analysis

Though the presented numerical model remains an idealized view of a multilayered geological system, the simulation can be computationally intensive and thereby time consuming (with a CPU time ranging from 5 to 30 min for a single run). Uncertainty analysis implies exhaustive simulations of multiple stochastic realizations and thus conducting such an analysis using the described numerical model appears too computationally constraining. A good alternative would be to replace the large scale complex numerical model by a simplified analytical model.

A first simplified analytical approach consists in assuming that the total stress state after injection remains constant to the remote total stress state *i.e.* the changes in the effective stresses correspond to the opposite of the changes in the pore pressure. A second approach consists in assuming a simplification of the reservoir geometry (*e.g.* Streit and Hillis [8] and Hawkes et al. [9]). In the idealized case of a thin, laterally extensive reservoir the vertical total stress is assumed equal to the remote total stress, whereas the horizontal total stress depends on Poisson's coefficient υ and on pore pressure change ΔP (*i.e.* the so-called "poroelastic effect").

$$\Delta\sigma_3 = \frac{(1-2\nu)}{1-\nu}\Delta P \tag{4}$$

2.4. Limitations of conventional analytical approaches

Rutqvist et al., [5] have shown that the described analytical approaches might lead either to an over- or to an underestimation of the maximal sustainable injection pressure. An additional comparison study is carried out here. The effective stresses at the interface of the reservoir and the caprock near the injection well are both estimated by the described numerical model and by both analytical models for various material and site configurations. Table 1 presents the ranges of value assumed for material properties in the context of the Paris basin.

Figure 2 presents the comparison between the numerically and analytically estimated tensile and shear slip failure criteria. The straight black line represents the first bisector. The closer the dots are from the straight line, the better the estimation is. It appears that both failure criteria are poorly estimated by conventional analytical models. The assumptions, on which the conventional analytical approach is based, appear too constraining for uncertainty analysis. Numerical analysis appears too computationally intensive for uncertainty analysis. An intermediate solution between both approaches should be proposed.

Table 1: Material Properties for the Paris Basin case

	Young Modulus [GPa]	Poisson coefficient [-]	Intrinsic permeability [m²]	Porosity [%]
Overburden	5 to 15	0.2 to 0.3	1.e-14 to 1.e-12	10 to 20
Caprock	5 to 20	0.2 to 0.3	1.e-21 to 1.e-16	1 to 5
Reservoir	10 to 25	0.2 to 0.3	1.e-14 to 25.e-12	10 to 20
Basement	25 to 50	0.2 to 0.3	1.e-18 to 1.e-16	1 to 5

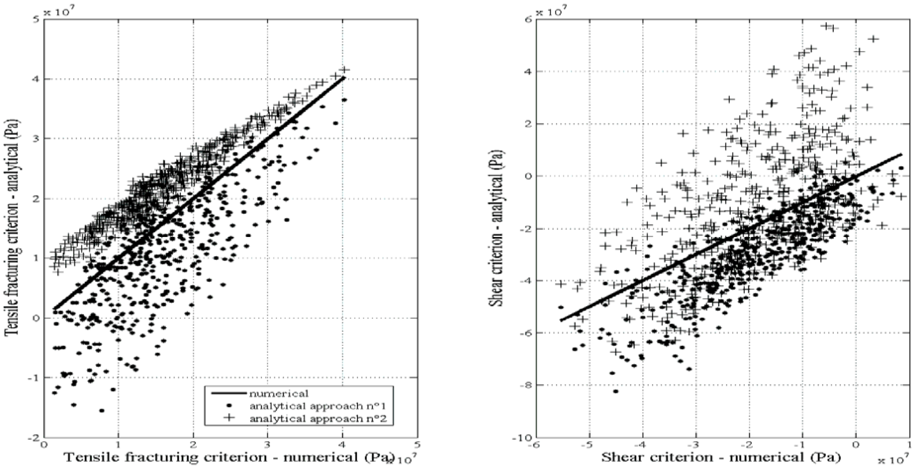

Figure 2: Comparison between numerically and analytically estimated cap rock tensile criteria (creation of vertical fracture with null tensile strength, left figure) and shear slip criteria (reactivation of cohesionless pre-existing fracture with internal friction angle of 30°, right figure)

3. A response surface strategy

An alternative approach is proposed in the framework of the response surface methodology. It consists in estimating at different reservoir depths the horizontal and vertical effective stresses (σ'_x ; σ'_y) as a linear combination of the input variables of the numerical model based on a finite range of large scale numerical deterministic simulations (section 2.2.). The main difficulty stems from the number of input variables of the numerical model (16 material parameters and 4 site specific parameters). A sensitivity analysis is then carried out to select the most influential variables of the numerical model (section 2.3.). The approximation quality of (σ'_x; σ'_y) is then assessed (section 2.4.) in a view to be used in a cap rock integrity assessment (section 4) using failure criteria.

3.1. Response surface method

The Response Surface Methodology (RSM) was first developed by Box and Wilson [2] and reads as follows. Given **y** the response, and **x** the vector of model variables such that $\mathbf{x} = [x_1, x_2,\dots, x_{nX}]$ with nX the number of model variables, the relationship between **y** and **x** is $\mathbf{y} = f(\mathbf{x})$. One may notice that in this paper, f is the hydraulical and geomechancial coupled finite element model described above. Since f has not a simple analytical form, a response surface g is created to approximate f (with ε represents a random error term). In this study, a first order polynomial *i.e.* linear regression is used as in Equation (5).

$$y = g(x) + \varepsilon = b_0 + \sum_{j=1}^{nX} b_j x_j + \varepsilon \qquad (5)$$

The objective is to determine the regression coefficients b_i, by means of a least squares regression analysis consisting in fitting the response surface approximations to a sample of the existing data. This sample provides a mapping between analysis inputs ($\mathbf{x}^i=[x^i_1, x^i_2,\ldots, x^i_{nX}]$) and analysis results (i.e., y^i). In this study, a random-based method, namely the Latin hypercube sampling method (McKay et al. [10]), is chosen to generate a homogeneous mapping of the input variables of the described numerical model. A sample of 100 simulations for each different reservoir depths (ranging from 1000m to 2000m) has been generated based on the value ranges of Table 1. It should be underlined that the value ranges of Table 1 represent the validity domain of the developed model.

3.2. Influential variables selection

Due to the large number of input variables of the numerical model (in total 20), a sensitivity analysis is conducted to identify the contributions of individual inputs to the uncertainty in analysis outcomes (Saltelli et al. [11]). The objective is to keep only the most important parameters in the response surface. In this view, a forward stepwise selection procedure is chosen. It operates in the following manner. The most influential variable is added to the model first producing a model of the form in equation (5) with one independent variable. Then the next most influential variable is added to the model producing a model of the form in equation (5) with two independent variables. The criterion for variable selection is the minimization of the root mean square error (denoted *RMSE*) based on the error between observed results (i.e. numerically calculated) and the estimated results. The process is continued in this manner until *RMSE* has reached an "acceptable" threshold.

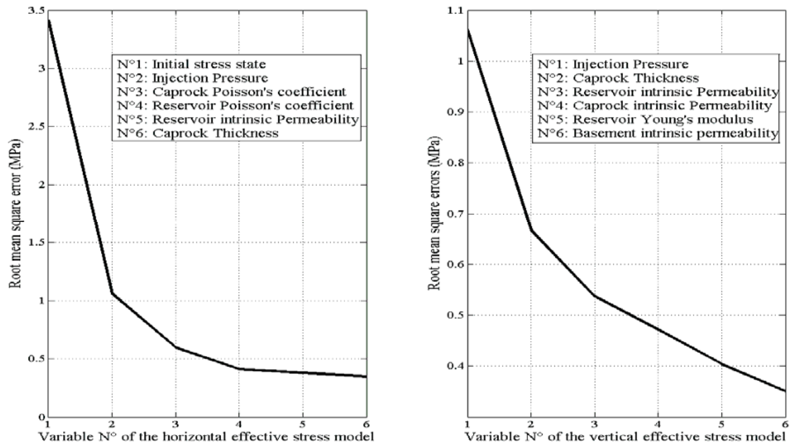

Figure 3: Variable selection according to the root mean square error for the estimation of the horizontal (left figure) and the vertical (right figure) effective stresses at reservoir depth of 1500m

Figure 3 presents the variable selection respectably for (σ'_x ; σ'_y) at depth 1500 m. The final *RMSE* for both stresses represent about 3.5 bars, which reaches less than 3 % of the mean of both effective stresses. This method is very informative to support decision in the field of CCS as it provides the decision maker with the most important site parameters i.e. the parameters on which the effort should be made to have sufficient knowledge.

3.3. Validation methodology

Once the regression coefficients have been determined for the most influential input variables, the quality of the model approximation should be validated in order to be used as a predictive model in the framework of an uncertainty analysis. The validation criterion is the cross-validation approach, which consists in estimating the robustness of the surrogate model *i.e.* how well the linear regression constructed from some training data is going to perform on future as-yet-unseen data. In this study, a "leave-one-out cross-validation" (*e.g.* Hjorth [12]) approach is chosen. The latter involves using a single observation from the original sample as the validation data, and the remaining observations as the training data. A linear regression is performed with the training data in order to predict the validation data. The square error between the approximation and validation data is then determined. This is repeated such that each observation in the sample is used once as the validation data. Based on the calculated square errors, the coefficient of determination (denoted R^2_{CV}) of the cross-validation is determined. It is defined as follows.

$$R^2_{CV} = \sum_{i=1}^{nS}(y_e - \mu)^2 \Big/ \sum_{i=1}^{nS}(y - \mu)^2 \qquad (6)$$

Where, y the true value, y_e the estimated value and μ the mean value of the sample. When the variation about the regression model is small, R^2_{CV} is close to 100 %, which indicates that the regression model is successful in matching the observed results. Table 2 shows the successful validation of the developed response surfaces.

Table 2: Cross validation results for the response surfaces

Depth [m]	1000	1250	1500	1750	2000
σ'x - R^2_{CV} [%]	99.1	99.5	99.0	99.3	99.4
σ'y - R^2_{CV} [%]	98.7	98.7	99.5	98.8	99.2

4. Uncertainty analysis in the cap rock integrity assessment, Paris Basin illustrative case

The effective stresses at different reservoir depths have been approximated with an acceptable quality and they can be used to estimate the cap rock failure criteria (equation 2 and 3). As the validated response surfaces are simple linear models, they can be easily used in an uncertainty analysis to support decision making in the field of CCS risk management. In this view, a two levels strategy is proposed.

4.1. Level one: Fist order estimate of maximal injection pressure

As the injection pressure is the parameter of the response surface, the maximal sustainable injection pressure can be evaluated using both failure criteria. Abacuses can be computed for a quick assessment of the maximal sustainable injection pressure regarding the site and material parameters identified in the sensitivity analysis (section 2.2.). Figure 4 illustrates such an abacus at depth 1500m for the tensile failure mechanism.

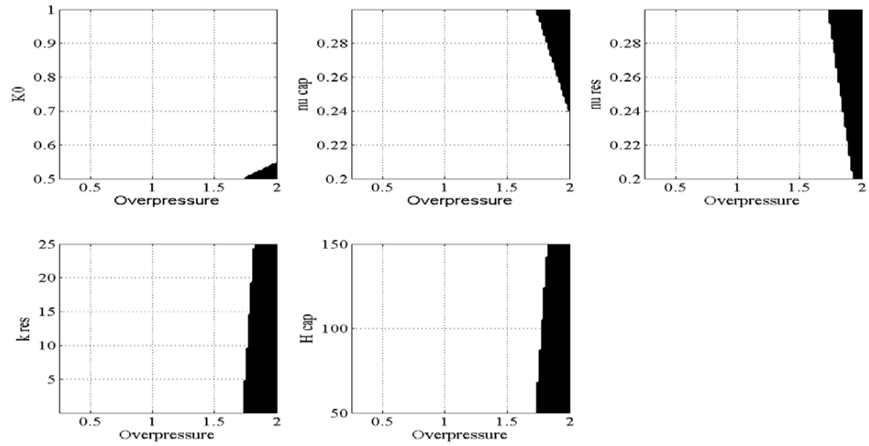

Figure 4: Abacus of the site parameters versus overpressure (in fraction of the initial pore pressure) for the tensile fracturing evaluation at depth 1500m – the damage zone is the black surface

It should be read as follows. Let consider a decision maker that is interested at injecting CO_2 with an overpressure twice the initial pore pressure. The abacus gives the minimal value of the initial stress state K_0 (*i.e.* 0.54) to prevent the cap rock to fracture (the damage zone is the black surface) considering that all other parameters (namely υ_{CAP} and υ_{RES}, k_{RES} and H_{CAP}) are taken in the most critical configuration (*i.e.* the configuration for which the tensile fracturing criterion is minimal). In the same manner, the minimal value for the Poisson's coefficient of the cap rock should reach at least 0.24 for the same overpressure. The critical values for the other parameters should be read following the same principle keeping in mind that the configuration is always chosen as the most critical one, thus implying that this first order evaluation remains a conservative estimate.

4.2. Level two: Epistemic and random uncertainties propagation

The uncertainty management developed in the methodological framework for determining safety criteria (Bouc et al. [1]) is based on the importance of separating uncertainties according to the nature of its source. Uncertainty can both results from a stochastic (e.g. natural variability resulting from heterogeneity) and from an epistemic source (e.g. imprecision resulting from the lack of information). Regarding the nature of uncertainty, a mathematical representation is more appropriate. A hybrid method (Guyonnet *et al.* [13]) is used to propagate both uncertainties using probability functions when sufficient data is available and intervals or fuzzy sets (seen as a set of confidence intervals) to represent imprecision (Zadeh [14]). More technical details can be found in Bellenfant and Guyonnet [15]. Table 3 gives the assumptions made in the Paris Basin case (based on Grataloup et al. [3]) for the uncertainty representation. The reservoir intrinsic permeability is a random parameter described by an empirical probability distribution (Rojas et al. [16]), whereas the other parameters are imprecise and represented by either simple intervals or triangular Fuzzy sets, which is defined by a most likely value (the "Core") and an interval of the most certain values (the "Support").

Table 3: Uncertainty representation in the Paris basin case

Variable		Nature of the uncertainty	Mathematical representation	Parameters
K0	[-]	epistemic	Triangular fuzzy set	Core {0.7}, Support [0.6 to 0.8]
υ cap& res	[-]	epistemic	interval	[0.2 to 0.3]
E res	[GPa]	epistemic	Triangular fuzzy set	Core {20}, Support [15 to 25]
H cap	[m]	epistemic	interval	[50 to 150]
k res	[m²]	random	Empirical probability distribution	Rojas et al. [16]
k cap	[m²]	epistemic	interval	[1.e-19 to 1.e-17]
k bas	[m²]	epistemic	interval	[1.e-18 to 1.e-16]

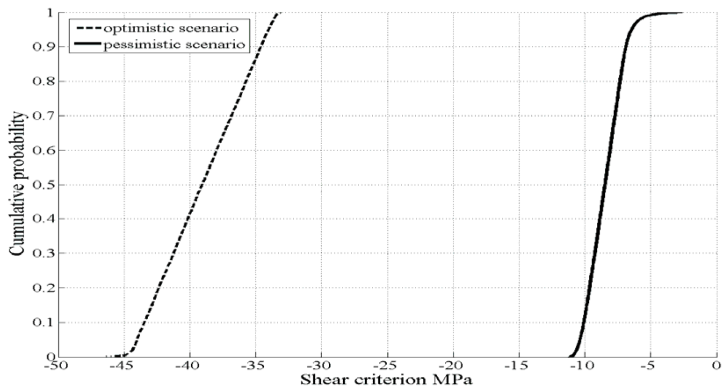

Figure 5: Uncertainties in the shear criterion at depth 1500 m for injection pressure of 2.5x the initial pore pressure

5. Conclusion

This paper presents a response surface methodology to develop simplified models to address uncertainties in cap rock integrity assessment to support decision making in the CO_2 storage risk management. The decision maker is provided with three main elements to be used for an informed CCS risk management: (1) the most important site parameters in the caprock failure analysis i.e. the parameters on which the effort should be made to have sufficient knowledge; (2) an analytical model of the effective stresses for a rapid assessment of the maximal sustainable injection pressure and (3) a simplified model to be used in a computationally intensive uncertainty analysis framework.

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